DELOCALIZATION IN CONTINUOUS DISORDERED SYSTEMS

M. Hilke[*] and J. C. Flores[†]

Université de Genève, Département de Physique Théorique, 24, Quai Ernest-Ansermet, CH-1211 Genève 4, Switzerland

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Continuous One-dimensional models supporting extended states are studied. These delocalized states occur at well defined values of the energy and are consequences of simple statistical correlation rules. We explicitly study alloys of δ-barrier potentials as well as alloys and liquids of quantum wells. The divergence of the localization length is studied and a critical exponent $2/3$ is found for the δ-barrier case, whereas for the quantum wells we find an exponent of 2 or $2/3$ depending on the well's parameters. These results support the idea that correlations between random scattering sequences break Anderson localization. We further calculate the conductance of disordered superlattices. At the peak transmission the relative fluctuations of the transmission coefficient are vanishing.

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INTRODUCTION

Recently the interest has increased substantially in order to find theoretical evidence for the breaking of Anderson localization by internal correlations in disordered systems[1−17]. For instance, in ref.[1] a tight-binding Hamiltonian with site correlations between the diagonal and the off-diagonal potentials was studied. A divergence of the localization length was obtained with a critical exponent $\nu = 2$ outside the band edges. In Refs.[2−6] a simple discrete model with correlations expressed by pairing (dimer) was studied. Their main result was the existence of a divergent localization length at some critical energies. In fact, this divergence is related to the existence of delocalized states found explicitly in ref.[7], which can be related to random phases and thus to extended states. Similar dimer models for classical systems were studied in ref.[8]. Using the inter-relation between a disordered Kronnig-Penney system and the dimer model (Poincaré map)[9−12] an infinite set of such delocalized states exist. The generalization of the dimer model to the N-mer case was considered, for instance, in refs.[13−16]. In this context perturbative methods were used in ref.[17].

In this way, delocalized states have been found 'contradicting' the usual belief that all eigenstates are localized in one-dimension (1-d). In fact, this is only apparent because the theorems related to localization in 1-d consider strictly uncorrelated random potentials (see for instance Ref.[18−22]). Interesting numerical simulations were carried out for binary disordered systems in ref.[23].

Usually these correlated disordered systems support delocalized states for well defined energies. In this respect, a 'band of delocalization' can be defined when the length L of the sample is smaller than the localization length $L_c(E)$, which diverges near the critical energy E_c. Quantitatively, the region of delocalization can be defined approximately, as

$$L < L_c(E) \sim \frac{1}{|E - E_c|^\nu}, \tag{1}$$

where ν has been determined explicitly in some models. Evidently this definition of a 'band of delocalization' is controversial because it depends on the existence of states in the interval $|E - E_c|$ and, moreover, is very different of the usual one related to true delocalized (unnormalizable) states. For instance, in the dimer model[2−4] a band of delocalized states is found to follow as $\Delta E \sim \sqrt{L}$, where L is proportional to the number of impurities N, nevertheless, the total number of states grows as L and therefore the relative number of delocalized states tends to zero as $1/\sqrt{L}$. It has been furthermore recently shown that additional perturbations on the dimer potentials lead to a suppression of these extended states[24]. Therefore these delocalization properties become more relevant in finite systems, as presented in the last part of this article. In quasi-one-dimensional systems, like models with dimerized interchain couplings[25], leading to a cantor-set-like conducting band, the finite temperature transmission can be greatly enhanced by the resonance energies.

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[*]Current address, Dpt. of electrical engineering, Princeton University, NJ-08544 Princeton, USA.
[†]Current address, Universidad de Chile FCFM Dept. de Física, casilla 487-3 Santiago, Chile.

As noticed, internal correlations break strong localization. In this paper we consider some simple models showing delocalization properties. For a general point of view we consider the one-dimensional disordered Hamiltonian of a particle in a random potential

$$H = \frac{p^2}{2m} + \sum_l V_l(x - x_l), \tag{2}$$

$$V_l(x) = \begin{cases} \neq 0 & -a_l < x < a_l \\ = 0 & \text{otherwise} \end{cases}, \tag{3}$$

thus, a sequence of scattering barriers centered at the random position x_l without overlap. Every barrier is symmetric with random support $2a_l$ and the distance between two barriers is given by

$$x_{l+1} - x_l = d_l, \tag{4}$$

which is a random quantity.

Between consecutive barriers the particle propagates freely and its wavefunction can be expressed as

$$\psi_l(x) = A_l e^{ikx} + B_l e^{-ikx} \quad \text{for} \quad x_l + a_l < x < x_{l+1} - a_{l+1}, \tag{5}$$

where k is the wavenumber related to the energy by $E = \hbar^2 k^2 / 2m$. Theoretical group arguments[26–28] relate the amplitudes (A_{l+1}, B_{l+1}) to (A_l, B_l) by means of

$$\begin{pmatrix} A_{l+1} \\ B_{l+1} \end{pmatrix} = \begin{pmatrix} e^{-ikx_l} & 0 \\ 0 & e^{ikx_l} \end{pmatrix} \begin{pmatrix} \alpha_l & \beta_l \\ \beta_l^* & \alpha_l^* \end{pmatrix} \begin{pmatrix} e^{ikx_l} & 0 \\ 0 & e^{-ikx_l} \end{pmatrix} \begin{pmatrix} A_l \\ B_l \end{pmatrix} \tag{6}$$

where the elements α, β of the collision matrix are inter-related like $|\alpha|^2 - |\beta|^2 = 1$ and we further on assume $\beta^* = -\beta$ (symmetric barrier). This form of the collision matrix is related to the fact that the time-independent Schrödinger equation is real.

Defining the wavefunction just after the collision with the l-th barrier as

$$\psi_l^+ = A_l e^{ik(x_l + a_l)} + B_l e^{-ik(x_l + a_l)}, \tag{7}$$

a condition of delocalization is

$$\psi_{l+1}^+ = \pm \psi_l^+, \tag{8}$$

which relates the elements of the collision matrix as

$$\alpha_l e^{ik(d_l + a_{l+1} - a_l)} + \beta_l^* e^{-ik(d_l + a_{l+1} + a_l)} = \pm 1. \tag{9}$$

The above delocalization condition is a sufficient one and, as expected, is not verified for totally uncorrelated systems. Condition (9) yields using $|\alpha|^2 - |\beta|^2 = 1$ the following simple delocalization condition

$$|\alpha_l| = 1 \quad \text{and} \quad \beta_l = 0, \tag{10}$$

which leads to $|A_{l+1}| = |A_l|$ and $|B_{l+1}| = |B_l|$.

Condition (9) inter-relates the random parameters like a_l and d_l in the disordered system and is therefore a source of correlation between these random parameters. In fact, in some simple systems, relations (9) and (10) can be satisfied and we present two examples: The δ-barriers-alloy and the quantum well liquid-alloy with interrelated random parameters.

To end this section, we remark that any relation similar to (6) can be formally written as a tight binding Schrödinger equation (Poincaré map) by considering

$$\hat{\alpha}_l = \alpha_l e^{ik(d_l + a_{l+1} - a_l)}, \quad \hat{\beta}_l = \beta_l e^{ik(d_l + a_{l+1} + a_l)} \tag{11}$$

and

$$D_{l+1}\psi_{l+1}^+ + D_l\psi_{l-1}^+ = V_l\psi_l^+, \tag{12}$$

where

$$D_l = \frac{D(k)}{2i(Im\hat{\alpha}_l - Im\hat{\beta}_l)} \quad \text{and} \quad V_l = \{D_{l+1}(\hat{\alpha}_l + \hat{\beta}_l^*) + D_l(\hat{\alpha}_{l-1}^* - \hat{\beta}_{l-1}^*)\}. \tag{13}$$

We notice that the above expression is only a formal one. For models such as the δ-barriers sequence, D_l is well defined for any k with the arbitrary choice $D(k) = 2i \sin k$. Nevertheless, in other systems singularities for some values of the wavenumber k can appear.

I. DELOCALIZATION IN A δ-BARRIER SEQUENCE

Consider a sequence of δ-potentials which are statistically distributed over lattice sites (alloy). Thus consider the sequence

$$V_l(x) = V_l\delta(x - x_l) \quad \text{and} \quad d_l = d, \tag{14}$$

where V_l are random uncorrelated parameters and d is a constant lattice parameter. In this case, the elements of the collision matrix are given by

$$\alpha_l = 1 + i\frac{V_l}{2k} \quad \text{and} \quad \beta_l = i\frac{V_l}{2k}. \tag{15}$$

The delocalization condition (9) becomes explicitly

$$e^{ikd} - \frac{V_l}{k}\sin(kd) = \pm 1. \tag{16}$$

In general, for any arbitrary momentum k, this condition does not hold because of the random quantity V_l. Nevertheless, if $k = n\pi/d$ ($n \in Z^*$), as first observed by Ishii[19], we have a set of delocalized states where $|\psi_{l+1}| = |\psi_l|$. This is at first sight very surprising because of the simplicity of the disordered model. Evidently, correlations exist and are related to the choice $d_l = d$ for any l. In fact, assuming a sample with N barriers, the usual $2N$ random parameters characterizing the uncorrelated system are reduced to N because of the constraint $d_l = d$.

In this model the physical interpretation is simple, in fact as long as $k = n\pi/d$ the electron does not 'feel' the random potential because the distance d, between consecutive barriers, is a multiple of its wavelength.

At this point, it is interesting to study the divergence of the localization length $L_c(E)$ near to the critical energy $E_c = \frac{1}{2m}(\frac{\hbar n\pi}{d})^2$. Using the Poincaré map (12) for this model we have

$$\psi_{l+1} + \psi_{l-1} = 2\{\cos kd\frac{V_l}{k}\sin kd\}\psi_l. \tag{17}$$

For $\epsilon = E_c - E \ll 1$ and $\hbar/2m$ taken as unity, equation (17) can be rewritten

$$\psi_{l+1} + \psi_{l-1} = \pm\left(2 - V_l\epsilon\frac{d^3}{n^2\pi^2}\right)\psi_l. \tag{18}$$

This last model was extensively studied in the limit $\epsilon \ll 1$ by Derrida and Gardner[29]. They calculated the complex Lyapounov exponent γ, where the real part corresponds to the inverse localization length and the imaginary part to π times the integrated density of states. Their results can be expressed as follows:

$$\begin{cases} Re(\gamma) \simeq K_1\epsilon^{2/3}\langle V_n^2\rangle^{1/3}\frac{d}{(n\pi)^{2/3}} \\ Im(\gamma) \simeq K_2\epsilon^{2/3}\langle V_n^2\rangle^{1/3}\frac{d}{(n\pi)^{2/3}}, \end{cases} \tag{19}$$

where $K_1 = 0.29\ldots$ and $K_2 = 0.16\ldots$ and $\langle\cdot\rangle$ is the average over all impurities. From (19) it is straightforward that the inverse localization length L_c^{-1} scales as

$$L_c^{-1} \sim \epsilon^{2/3}\langle V^2\rangle^{1/3} \tag{20}$$

and the density of states is

$$\rho(\epsilon) = \partial_\epsilon Im\gamma(\epsilon) \sim \epsilon^{-1/3}. \tag{21}$$

The main result of this section is to show that a continuous disordered model where the potential amplitudes are random but placed on a lattice, exhibits extended states for discrete values of the energy. We recall that for this model the result was first pointed out by Ishii[19]. However, the exponent 2/3 we obtain is different to the 1/2 obtained by Ishii, who considered a Cauchy distribution. The correlation in this model comes from the fact that the impurities are placed on a regular lattice. This in fact is a very natural physical assumption, as one can imagine an alloy where different atoms are placed randomly, described by the random amplitude of the potential, but on a lattice. This system would lead to a similar model studied above. In fact the models where the locations of the impurities are continuously random, no extended states have been found so far for delta like potentials. For finite potentials they do exist as we will mention in the next section.

II. DELOCALIZATION IN A QUANTUM WELL SEQUENCE

The case of delta impurities considered in the previous section is very special and cannot be used in order to describe more general impurity potentials. This is why it is of interest to study other types of potentials, which could eventually describe more general impurity potentials. One of the simplest examples of such a potential is the rectangular well potential. In principle one could approximate any potential with rectangular wells if the elementary width is small enough. Therefore we will restrict our considerations to rectangular well potentials.

As an important result we observe the existence of extended states for systems where we have continuous spatial disorder and discrete shape disorder. This has to be contrasted with the case of delta impurities where extended states exist only when we have shape disorder alone, i.e., where the amplitudes of the impurity potentials are random.

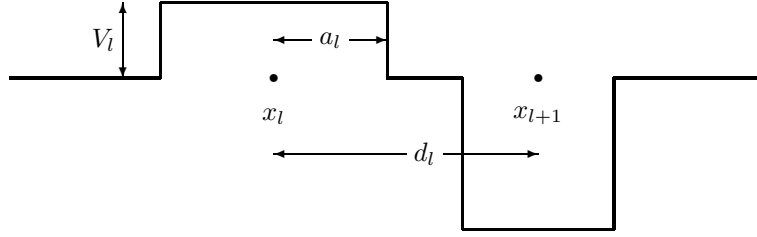The aspect and definitions of the rectangular well potential are shown in fig. 1:

FIG. 1. Rectangular well potentials

For this case we have

$$\alpha_l = \frac{e^{-i2a_l k}}{2 p_l k} \left(2 p_l k \cos(2 a_l p_l) + i (p_l^2 + k^2) \sin(2 a_l p_l) \right) \tag{22}$$

and

$$\beta_l = i \frac{(p_l^2 - k^2) \sin(2 a_l p_l)}{2 p_l k}, \tag{23}$$

where $p_l = \sqrt{|k^2 - V_l|}$. We have to point out that these results are only valid when $E \geq V_l$. For the case $E \leq V_l$ we have to replace $cos(\cdot)$ and $sin(\cdot)$ in (22,23) by their hyperbolic counterparts.

Using the delocalization condition (10) we have an extended state when $\beta_l = 0$, thus

$$E = k^2 = V_l + \frac{n_l^2 \pi^2}{4 a_l^2} \quad \text{with } n_l \text{ an integer.} \tag{24}$$

This means that if we have a discrete set of impurity configurations, we have critical energies E_c at which the states are delocalized. The impurities have just to be constructed with the help of equation (24) once we replace E by E_c, where we can take different values for V_l or a_l by changing n_l. A *very remarkable* aspect of these disordered models is that they are *independent* of the space disorder expressed by d_l as was already appreciated by Tong[30] for a different model.

We evaluate the exponent for the following case: suppose $d_l = d$ and $a_l = a$, i.e., we are left with a pure shape disorder. Let $k_c^2 = E_c$ be the critical energy defining the correlation (24) of the disorder and writing the Poincaré map (12) around $k = k_c + \epsilon$, with ϵ very small, we obtain

$$\psi_{l+1} + \psi_{l-1} = \{2 \cos(k_c(d - 2a)) + \epsilon \xi_l\} \psi_l, \tag{25}$$

where ξ_l is random and function of V_l. For the case where $k_c(d - 2a)/\pi$ is an integer we obtain the same result as for the delta-barrier case (18-21), thus $\nu = 2/3$. When $k_c(d - 2a)/\pi$ is not an integer we can also use Derrida and Gardner's[29] result for the case inside the band, yielding $\nu = 2$. The most general case, where d_l and a_l are random, and when no particular configuration is used, we obtain numerically the exponent $\nu = 2$.

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The interesting aspect of these continuous disordered systems is that they can describe a real physical situation of electrons in a certain potential. The problem with continuous models is that the expressions of the transfer matrices can be much more complicated except if one considers delta impurities or rectangular well potentials. For more general impurity potentials one can either approximate them with a sum of rectangular barriers or use the semiclassical WKB approximation. This last approximation can, however, have dramatic effects on the localization properties, especially around some critical energies, as they are very sensitive to small perturbations.

Summerizing the localization length divergences for the δ-impurity and quantum wells we have:

$$L_c(E) \sim \frac{1}{|E - E_c|^{\nu}} \ , \ \text{where} \ \nu = \begin{cases} = 2/3 & \delta\text{-barrier and } k_c(d - 2a)/\pi \text{ an integer for the quantum well} \\ = 2 & \text{otherwise} \end{cases} \tag{26}$$

III. FLUCTUATIONS AND CONDUCTANCE

In one dimensional disordered systems, the relative fluctuations of the transmission coefficients diverge with the size of the system[28]. Therefore the average transmission is a bad statistical quantity. However at the critical energies discussed above, the states are deterministic and therefore one would expect no fluctuations. In the following we evaluate the relative fluctuations explicitly and calculate the conductance for superlattices around these critical energies.

Around the critical energy E_c we evaluated the localization length dependence on energies, therefore $T_N \sim e^{-L/L_c}$, where T_N is the transmission coefficient after N barriers and N is proportional to L. The relative fluctuations are then given by

$$\frac{\Delta T}{T} \sim N \frac{\Delta L_c}{L_c^2}. \tag{27}$$

Using the central limit theorem, valid for the logarithm of the product of random determinant one matrices, the relative fluctuations of the localization length can be expressed as

$$\frac{\Delta L_c}{L_c} \sim N^{-1/2}, \tag{28}$$

hence using (26-28)

$$\frac{\Delta T}{T} \sim N^{1/2}|E - E_c|^{\nu}. \tag{29}$$

In usual one-dimensional disordered systems the average distance between eigenvalues is of the order N^{-1}, therefore using $|E - E_c| \sim N^{-1}$, we obtain

$$\frac{\Delta T}{T} \sim |E - E_c|^{\nu - 1/2}. \tag{30}$$

This demonstrates that for the case of interest here, both cases $\nu = 2$ and $\nu = 2/3$ have vanishing relative fluctuations near the critical energies. This fluctuation analysis gives also a bound on the possible divergence exponent ν. In fact as long as $\nu > 1/2$, the average transmission around the critical energies is a good statistical quantity.

Many physical systems can be very well approximated with either rectangular well potentials or delta potentials. This is the case for superlattices of heterostructures. One can grow very precise, up to the atomic precision, layers of $GaAs$. Then one dopes differently one layer with Al and then again the same layer and one obtains in this way a single so called delta doped layer. This can then be repeated as often as one wishes. This last structure is very well described in the direction of the layers by delta impurity models. Instead of doping differently only one layer we can also dope a finite number of layers differently. In this case the potential looks more like a rectangular well potential, where the amplitude depends on the concentration of the doping used. In this way it is possible to grow one-dimensional quantum wires where both directions of the layers are etched, two-dimensional systems where only one of the direction of the layers is etched and finally three-dimensional systems.

The two probe conductance is simply given by the sum of the transmission coefficients[31], thus

$$G(\mu) = \sum_{k|E=\mu} T(k) \cdot \frac{e^2}{h}, \tag{31}$$

where μ is the chemical potential.

For a one-dimensional quantum wire the conductance is just given by the transmission coefficient, as there is only one conducting channel. Around the critical energies we evaluated the localization length dependence on energies, therefore using $T_N \sim e^{-N/L_c}$, where T_N is the transmission coefficient after N barriers, we obtain conductance peaks at the critical energies of the form

$$G(\mu) \sim e^{-\gamma|\mu - E_n|^{\nu}}, \tag{32}$$

where μ is the chemical potential, γ depends on the size and disorder of the system and E_n are the critical energies. For the delta doping $E_n = \frac{1}{2m}(\frac{\hbar n\pi}{d})^2$ and $\nu = 2/3$. For the rectangular case we have one critical energy E_c and the random Al doping potentials are given by

$$V_l = E_c - \frac{n_l^2 \pi^2}{a^2} \quad \text{with } n_l \text{ a random integer} \tag{33}$$

and a is the width of the doped layers. The width d_l of the undoped layers can be random and we obtain $\nu = 2$. For the special case where $d_l = d$ is constant the value of the exponent ν depends on the ratio $E_c(d - 2a)^2/\pi^2$. If this ratio is an integer the exponent is $\nu = 2/3$ but remains $\nu = 2$ otherwise. The interesting feature of this system, is that it would behave as a perfect filter. The band-width could be controlled by the size or γ and the desired critical energy by the choice of dopants.

In order to evaluate the conductance of the three-dimensional system, as defined above, we have to sum over all possible channels. In the directions (x,y) perpendicular to the grown layers the density of states is simply the usual box filling density. In the infinite limit we have to integrate over the Brillouin zone which yields,

$$G \sim \int_{k_x^2 + k_y^2 \leq \mu} e^{-\gamma|\mu - k_x^2 - k_y^2 - E_c|^{\nu}} dk_x dk_y \tag{34}$$

The plots of the conductance from eq. (34) as a function of the chemical potential are given in fig. 2 for different system sizes characterized by γ and for the two cases $\nu = 2$ and $\nu = 2/3$.

The two-dimensional case is presented in fig. 3. In this case the behavior is consequently different for $\nu = 2$ and $\nu = 2/3$. Indeed for $\nu = 2/3$ we have a singular derivative, which could be observed experimentally, in order to distinguish between the two cases.
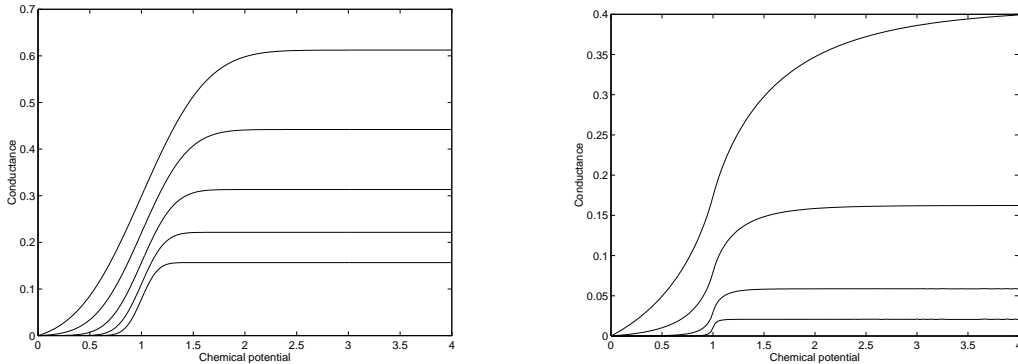

FIG. 2. Conductance for $\nu = 2$ and $\nu = 2/3$ (right graph) as a function of the chemical potential, for the case where the resonance energy is $E_c = 1$. The different curves represent different values of $\gamma = 2^n$, with $n = 1, 2, 3, 4, 5$. The uppermost curve represents the case $\gamma = 2$.
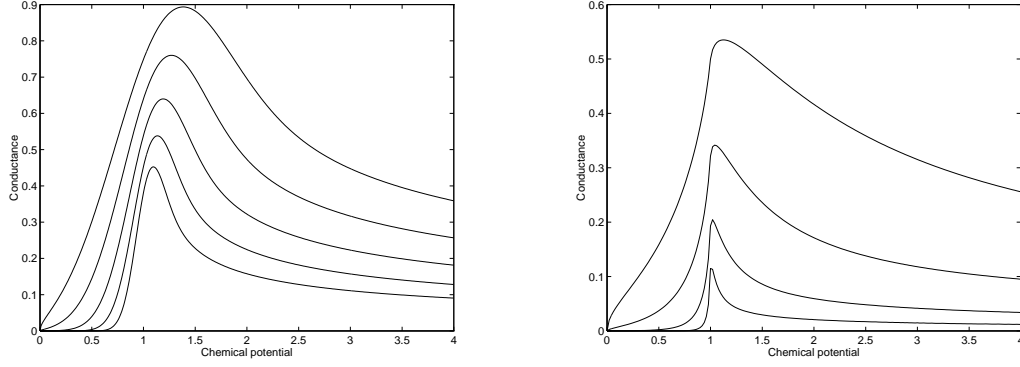
FIG. 3. Conductance for the two-dimensional case with the same parameters as in fig. 2.

The quantitative values can also be estimated. In the delta doping case the typical Fermi wavelength is of the order of 200Å and the typical layer thickness is of the order of 5Å. This means that we have to construct delta doped layers with around 40 layers in between. In order to obtain the disorder we just have to chose randomly the dopant or the concentration of the doping for the delta layers. The same reasoning can be held for rectangular potentials, where one just has to chose a particular potential configuration.

CONCLUSIONS

In the first section we demonstrated the existence of extended states in continuous disordered systems with delta impurities placed on a lattice and obtained for the exponent describing the divergence of the localization length $\nu = 2/3$. This model hence demonstrates the existence of extended states in systems with only shape disorder. In the second section, using rectangular potentials we demonstrated that models with shape *and* space disorder can also exhibit extended states. The only constraint on the disorder distribution is that it must be discrete for the shape disorder but can be continuous for the space disorder. In this case the correlation in disorder leading to the existence of delocalized states is simply the fact that the distribution mentioned above is discrete and obeys relation (24). Therefore one has to be very careful when one discusses disordered systems using discrete disorder distributions as there can exist singularities in the spectrum. The exponents of the localization length divergence are very interesting. In fact, depending on the parameters of the quantum wells we obtain different exponents, either $\nu = 2/3$ or $\nu = 2$.

The relative fluctuations of the conductance around these critical energies are vanishing. Therefore the conductance is a well defined statistical average and represents the transport properties of these disordered systems.

Acknowledgements

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